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1,4-Polymerization of Butadiene with Cationic
 $[\text{Ni}^{\text{II}}(\text{C}_4\text{H}_7)(\text{C}_4\text{H}_6)\text{PH}_3]^+$ Complexes

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published in

Modern Methods and Algorithms of Quantum Chemistry,
J. Grotendorst (Ed.), John von Neumann Institute for Computing,
Jülich, NIC Series, Vol. 2, ISBN 3-00-005746-3, p. 9, 2000.

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Density Functional Study of the 1,4-Polymerization of Butadiene with Cationic $[\text{Ni}^{\text{II}}(\text{C}_4\text{H}_7)(\text{C}_4\text{H}_6)\text{PH}_3]^+$ Complexes.

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According to the π -allyl-insertion mechanism¹ the entire catalytic cycle of 1,4-polymerization of butadiene has been theoretically studied by employing a gradient-corrected density functional method with the cationic butenylbis(ligand) complexes as the catalyst.² We have investigated competitive chain propagation cycles for generation of a cis-1,4- and trans-1,4-polymer, and also anti-syn isomerization. The calculations provide a clear insight into the stereoregulation mechanism of trans-1,4 polymerization.

¹ Taube, R.; Gehrke, J.-P.; Böhme, P. *Wiss. Zeitschr. TH Leuna-Merseburg* **1987**, 39, 310.

² Tobisch, S.; Bögel, H.; Taube, R. *Organometallics* **1998**, 17, 1177.